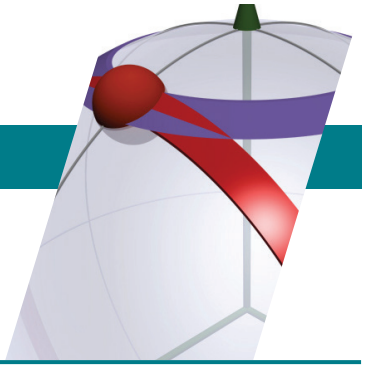
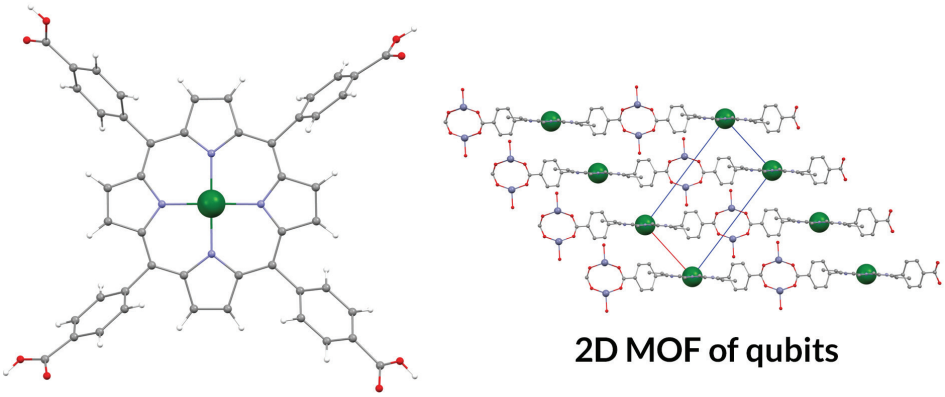


MATERIALS SCIENCES

A 2D Lattice of Molecular Qubits for Quantum Computing



Left: A promising vehicle for the realization of a quantum bit of information, or qubit, is the Cu(II) porphyrin molecule (Cu=green, N=blue, O=red, C=gray, H=white). The Cu(II) spin provides the two-level system capable of encoding quantum information. Right: Structure of the 2D metal-organic framework (MOF) formed upon reaction with Zn(II) ions, as determined by measurements at ALS Beamline 11.3.1.

Scientific Achievement

Researchers developed a way to build a 2D lattice of molecular-spin qubits (quantum bits of information), with control over qubit orientation and localization.

Significance and Impact

The work enables the integration of molecular quantum-information hardware into the scalable, robust, solid-state architectures needed for performing quantum computation.

Hardware for a quantum computer

Quantum computing is a hot topic these days for good reason: if realized, quantum computers could solve problems that are quantitatively and qualitatively beyond what's possible with today's classical computers. By harnessing phenomena such as wave-function superposition, a quantum computer could tackle otherwise intractable problems from cryptography and financial modeling to artificial intelligence and the simulation of quantum-realm chemical and nanotech systems.

While computer scientists are developing the necessary software, materials scientists are working on hardware. The two quantized electron-spin orientations of a magnetic molecule form a natural two-level quantum system that could provide the basis for encoding the states of a quantum bit of information, or qubit. This approach facilitates scalability, in that extremely large numbers of identical qubits could be obtained in one reaction. However, it also requires the ability to maintain control over both the positions and orientations of the molecules in a solid-state device, something that previous research involving isolated molecules on surfaces had suggested would be difficult.

A 2D nanosheet with porphyrin qubit nodes

In this work, researchers hypothesized that the required control could be enforced through the periodicity of 2D metal–organic frameworks (MOFs) with molecular qubits forming the nodes. These nodes would consist of porphyrins: ring-shaped organic molecules with metal ions at their centers. Specifically, they focused on Cu(II) porphyrin molecules (CuTCPP) that connect through four coordinating carboxylic acid groups.

The targeted 2D MOF with a square grid of regularly spaced and homogeneously oriented porphyrin nodes was successfully formed by reaction with diamagnetic Zn(II) ions. Single-crystal x-ray diffraction measurements at ALS Beamline 11.3.1 allowed the determination of the solid-state structure of the 2D MOF. Due the challenging size and intrinsic stacking of the available crystals, this was only possible thanks to the ALS's unique capabilities in small-molecule crystallography (now at Beamline 12.2.1).

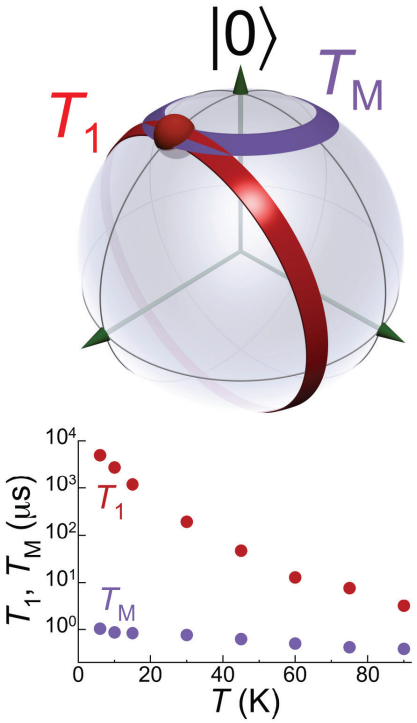
The quantum coherence of the CuTCPP molecule was evaluated both isolated and as a node in the MOF. The molecule exhibited long spin-lattice relaxation times (T_1) and phase-memory times (T_M), on the order of milliseconds, indicating that CuTCPP is a valid qubit candidate and, more importantly, that its quantum coherence is maintained upon insertion into the 2D framework.

Toward integration into hybrid architecture

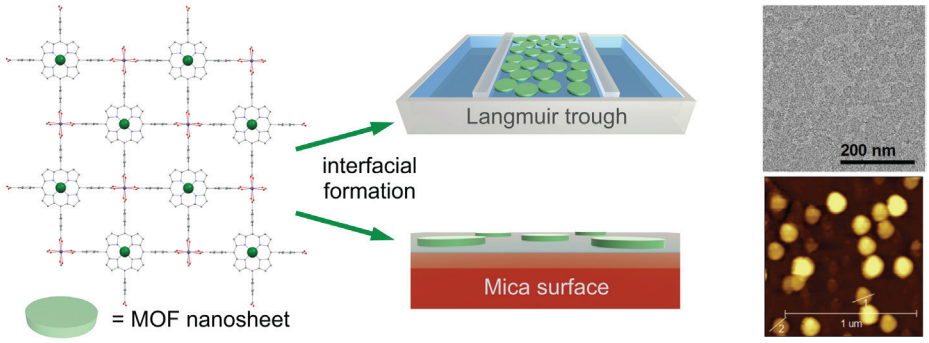
The researchers also demonstrated that monolayer nanodomains of the 2D MOF are readily formed at an air-water interface. A controlled number of layers of these nanodomains can then be transferred to a variety of substrates, preserving the homogeneity and orientation of the CuTCPP molecules, as confirmed through in situ grazing-incidence x-ray scattering (GIXS) performed at SOLEIL Synchrotron and electron paramagnetic resonance.

Eventually a protocol was developed allowing the direct, in situ formation of qubit-rich nanodomains over a mica substrate that mimics the oxide-layer surfaces found in classical solid-state devices. Topographic observations and local chemical analyses confirmed that similar isolated nanodomains were formed at microscopically selected locations.

Overall, the work demonstrates the potential of a framework approach toward the integration of molecular qubits onto solid surfaces with controlled localization and enforced orientation. Future developments should involve the downsizing of localization control to tens of nanometers, which would be necessary to construct hybrid (classical/quantum) processors.



Top: A Bloch sphere is a useful geometrical representation of a two-level quantum mechanical system. The north and south poles typically represent the two base states (e.g., 0 and 1). Superpositions of those two states are represented by points on the surface of the sphere. Two figures of merit for a quantum-computing system are the spin-lattice relaxation time (T_1) and phase-memory time (T_M), corresponding to a loss of information about the superposition amplitude θ and phase ϕ, respectively, as indicated by the red and purple circles. Bottom: T_1 and T_M determined for the CuTCPP nodes in the 2D MOF (diluted to 1% with ZnTCPP).



Left: Structure of the square-grid MOF nanosheet similar to those in the bulk solid material that form at the air-water interface either in a Langmuir trough (a set-up used to form and deposit single or multiple monolayers on a solid substrate) or on mica surfaces. Right: Transmission electron microscope (TEM) image of the MOF nanosheets formed in a Langmuir trough and atomic-force microscope (AFM) image of the same nanosheets formed locally on mica.

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